Investigation into Nonlinear Grasshoff Number Dependence of Convection within a Hot Melt during Directional Solidification

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by

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Abstract: The motivation behind this study derives from the demand within industry for bimetallic crystals of minimal defect in constituent distribution. One method of growing such crystals is to draw the molten mixture through an enclosed ampoule in a Bridgman furnace, and is a good technique for the production of Gallium Arsenide and other semiconductors. The current difficulty with this production method is the radial segregation of the constituents within the crystal caused by the formation of convective currents within the melt during cooling. Experimental and numerical evidence suggests that this convection takes the form of a single large eddy, the magnitude of which appears to vary linearly with Gr, even for large Gr where nonlinear effects should become important. In order to better understand, and possibly explain, this phenomenon, a mathematical model was used.

Introduction

The Bridgman production method involves drawing the crystal constituents through a furnace in order to create a uniform melt. This melt is then drawn through a tube and allowed to cool such that the rate of crystal growth is equal to the speed at which the ampoule is drawn through the tube. This allows the interface between the crystal and the melt to be maintained at a constant position within the tube. For more detailed information on the physical problem and Bridgman furnace crystal production methods reference (Adornato and Brown[1] 1987) Temperature gradients, within the melt above the crystal interface, drive the convection currents which lead to radial segregation of the constituents within the crystal. This study will model the region above the crystal interface as defined in figure 1, below.

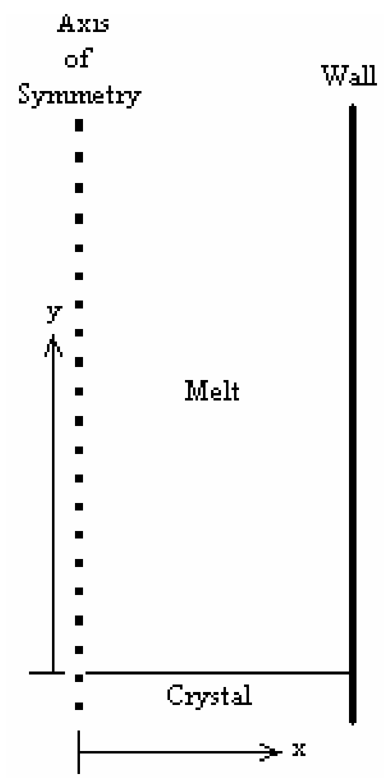

Fig 1
Model of Region being studied

The model in figure 1, reflects the assumption of an axisymmetric container, allowing the problem to be modeled as a 2 dimensional planar flow field over the domain $x = [0,1]$ and $y = [0,\infty)$. The non-dimensionalized governing equations for this case are,

$$\nabla^2 q = \Pr(uq_x + vq_y) \tag{1}$$

$$\nabla^2 w + Grq_x = (uw_x + vw_y) \tag{2}$$

$$\nabla^2 y = -w \tag{3}$$

Where, $\Pr = \dfrac{u}{a}$ $\qquad$ $Gr = \dfrac{a^2 agq_x}{u^2}$

The boundary conditions for this problem are:

<u>Along wall</u> $(x = 1)$

$$y = 0 \qquad w = 0 \qquad q_x = be^{-by} \tag{bc1}$$

<u>Along axis of symmetry</u> $(x = 0)$

$$y = 0 \qquad w = 0 \qquad q_x = 0 \tag{bc2}$$

<u>Along crystal interface</u> $(y = 0)$

$$y = 0 \qquad y_y = 0 \qquad q_x = 0 \tag{bc3}$$

<u>Limit as</u> $(y \to \infty)$

$$y = 0 \qquad w = 0 \qquad q_x = 0 \tag{bc4}$$

Boundary condition (bc1) has been chosen such that the total heat flux across the boundary *x=1*, is constant regardless of the value of b. It is also important to note the use of an $w = 0$ boundary condition at the wall. Previous work (Izadnegahdar[2] 2004) on this problem utilized $u = v = 0$ as the wall boundary condition in solving a similar model. It has, however, been shown (Tanveer[3] 1994,Foster[4] 1997) that replacing the no slip condition with an $w = 0$ condition at the wall has little effect on the behavior of the flow near the crystal interface.

Typically, in semiconductor melts, thermal conductivity dominates viscous diffusion, resulting in Prandtl numbers on the order of 10^{-3} to 10^{-2} (Kim[5] 1996). For this reason the Prandtl number will be set to zero for this investigation. With Prandtl number set to zero, equation (1) becomes simply,

$$\nabla^2 q = 0 \tag{4}$$

The Grasshoff number is, however, quite large for this case. Previous numerical work on this issue has found that the vorticity varies linearly with Gr up to values of order 10^3. While this trend makes sense for small Grasshoff numbers, the fact that *u*, *v*, and w are all proportional to Gr, means that the right hand side of equation (2) should be proportional to Gr^2. Thus the linear relation between vorticity and Gr should not hold for large values of Gr.

In order to resolve this apparent contradiction, this study will attempt to solve for the flow field at small Grasshoff number by approximating w and y as power series in Gr.

$$w = w_0 Gr + w_1 Gr^2 + w_2 Gr^3 + w_3 Gr^4 + \ldots$$

$$y = y_0 Gr + y_1 Gr^2 + y_2 Gr^3 + y_3 Gr^4 + \ldots$$

Substituting into equations (2) and (3), and equating powers of Gr, the following relations are attained.

$$\nabla^2 w_0 = -q_x \tag{5}$$

$$\nabla^2 w_1 = y_{0y} w_{0x} - y_{0x} w_{0y} \tag{6}$$

$$\nabla^2 y_0 = -w_0 \tag{7}$$

$$\nabla^2 y_1 = -w_1 \tag{8}$$

Temperature Gradient

From equation (4),

$$\nabla^2 q = 0$$

Then by taking an x derivative, a relation for the temperature gradient is obtained.

$$\nabla^2 q_x = 0 \tag{9}$$

The general form of the solution is given by,

$$q_x = xbe^{-by} + \sum_{n=1}^{\infty} A_n \sin(npx) \tag{10}$$

By substituting, (10) into (9),

$$\sum_{n=1}^{\infty} \left(A_n'' - n^2 p^2 A_n \right) \sin(npx) = -xb^3 e^{-by} \tag{11}$$

Also, the sine series representation of $-x$ is,

$$-x = \sum_{n=1}^{\infty} \frac{2}{np} (-1)^n \sin(npx)$$

Equation (11) can therefore be written as,

$$\sum_{n=1}^{\infty} \left(A_n'' - n^2 p^2 A_n \right) \sin(npx) = \sum_{n=1}^{\infty} \frac{2}{np} (-1)^n b^3 e^{-by} \sin(npx)$$

Then by equating coefficients, a differential equation in A_n is obtained,

$$A_n'' - n^2 p^2 A_n = \frac{2}{np} (-1)^n b^3 e^{-by} \tag{12}$$

The general solution for A_n is,

$$A_n = \frac{2(-1)^n b^3}{np\left(b^2 - n^2 p^2\right)} e^{-by} + C_n e^{-npy}$$

Thus,

$$q_x = xbe^{-by} + \sum_{n=1}^{\infty}\left(\frac{2(-1)^n b^3}{np\left(b^2 - n^2p^2\right)}e^{-by} + C_n e^{-npy}\right)\sin\left(npx\right) \qquad (13)$$

Imposing boundary condition (bc3) on (13),

$$0 = -\sum_{n=1}^{\infty}\frac{2}{np}\left(-1\right)^n b\sin\left(npx\right) + \sum_{n=1}^{\infty}\left(\frac{2(-1)^n b^3}{np\left(b^2 - n^2p^2\right)} + C_n\right)\sin\left(npx\right)$$

Then by equating coefficients,

$$\frac{2}{np}\left(-1\right)^n b = \frac{2(-1)^n b^3}{np\left(b^2 - n^2p^2\right)} + C_n$$

Therefore,

$$C_n = \frac{-2(-1)^n npb}{b^2 - n^2p^2}$$

The complete solution for the temperature gradient is then,

$$q_x = xbe^{-by} + \sum_{n=1}^{\infty}\frac{2(-1)^n}{np}\left(\frac{b^3}{b^2 - n^2p^2}e^{-by} - \frac{n^2p^2b}{b^2 - n^2p^2}e^{-npy}\right)\sin\left(npx\right) \qquad (14)$$

Solution for w_0

With the solution for q_x known, w_0 can be found from equation (5).

$$\nabla^2 w_0 = -q_x$$

Let w_0 be represented by the infinite series,

$$w_0 = \sum_{n=1}^{\infty} (G_n) \sin(npx)$$

Equation (14) can be rewritten in the form,

$$q_x = \sum_{n=1}^{\infty} g_1 \left(e^{-by} - e^{-npy}\right) \sin(npx) \qquad g_1 = \frac{2(-1)^n npb}{b^2 - n^2p^2}$$

Equation (5) can then be rewritten as,

$$\sum_{n=1}^{\infty} \left(G_n'' - n^2p^2 G_n \right) \sin(npx) = \sum_{n=1}^{\infty} g_1 \left(e^{-npy} - e^{-by}\right) \sin(npx) \tag{15}$$

Equating coefficients to arrive at a differential equation in G_n,

$$G_n'' - n^2p^2 G_n = g_1 \left(e^{-npy} - e^{-by}\right) \tag{16}$$

The general solution of (16) is,

$$G_n = C_{n1} e^{-npy} - \frac{g_1}{2np} y e^{-npy} - \frac{g_1}{b^2 - n^2p^2} e^{-by}$$

The general solution for the w_0 is then,

$$w_0 = \sum_{n=1}^{\infty} \left(C_{n1} e^{-npy} - \frac{g_1}{2np} y e^{-npy} - \frac{g_1}{b^2 - n^2p^2} e^{-by} \right) \sin(npx) \tag{17}$$

Solution for y_0

The relation between the stream function, y_0, and w_0 is given by (7),

$$\nabla^2 y_0 = -w_0$$

Let y_0 be represented by the infinite series,

$$y_0 = \sum_{n=1}^{\infty} (F_n) \sin(npx)$$

Then,

$$\sum_{n=1}^{\infty}\left(F_n'' - n^2p^2F_n\right)\sin(npx) = -\sum_{n=1}^{\infty}\left(C_{n1}e^{-npy} - \frac{g_1}{2np}ye^{-npy} - \frac{g_1}{b^2 - n^2p^2}e^{-by}\right)\sin(npx)$$

Equating coefficients to attain a differential equation in F_n,

$$F_n'' - n^2p^2F_n = \frac{g_1}{2np}ye^{-npy} + \frac{g_1}{b^2 - n^2p^2}e^{-by} - C_{n1}e^{-npy} \tag{18}$$

The general solution of (18) is,

$$F_n = \left[C_{n2} + \left(\frac{C_{n1}}{2np} - \frac{g_1}{8n^3p^3}\right)y - \left(\frac{g_1}{8n^2p^2}\right)y^2\right]e^{-npy} + \frac{g_1}{\left(b^2 - n^2p^2\right)^2}e^{-by}$$

The general solution for y_0 is then,

$$y_0 = \sum_{n=1}^{\infty}\left(\left[C_{n2} + \left(\frac{C_{n1}}{2np} - \frac{g_1}{8n^3p^3}\right)y - \left(\frac{g_1}{8n^2p^2}\right)y^2\right]e^{-npy} + \frac{g_1}{\left(b^2 - n^2p^2\right)^2}e^{-by}\right)\sin(npx) \tag{19}$$

According to boundary condition (bc3), $y_0|_{y=0} = 0$, which leads to,

$$C_{n2} = -\frac{g_1}{\left(b^2 - n^2p^2\right)^2}$$

y_0 then becomes,

$$y_0 = \sum_{n=1}^{\infty}\left(\left[\left(\frac{-g_1}{\left(b^2-n^2p^2\right)^2}\right)+\left(\frac{C_{n1}}{2np}-\frac{g_1}{8n^3p^3}\right)y-\left(\frac{g_1}{8n^2p^2}\right)y^2\right]e^{-npy}+\frac{g_1}{\left(b^2-n^2p^2\right)^2}e^{-by}\right)\sin(npx)$$

The boundary condition (bc3), $\left.\frac{\partial y_0}{\partial y}\right|_{y=0} = 0$ requires,

$$0 = \frac{npg_1}{\left(b^2-n^2p^2\right)^2}+\frac{C_{n1}}{2np}-\frac{g_1}{8n^3p^3}-\frac{g_1 b}{\left(b^2-n^2p^2\right)^2}$$

Therefore,

$$\frac{C_{n1}}{2np}-\frac{g_1}{8n^3p^3}=\frac{g_1(b-np)}{\left(b^2-n^2p^2\right)^2}$$

y_0 then becomes,

$$y_0 = \sum_{n=1}^{\infty}\left(\left[\left(\frac{-g_1}{\left(b^2-n^2p^2\right)^2}\right)+\left(\frac{g_1(b-np)}{\left(b^2-n^2p^2\right)^2}\right)y-\left(\frac{g_1}{8n^2p^2}\right)y^2\right]e^{-npy}+\frac{g_1}{\left(b^2-n^2p^2\right)^2}e^{-by}\right)\sin(npx)$$

Or by substituting in g_1,

$$y_0 = \sum_{n=1}^{\infty}\frac{-2(-1)^n npb}{\left(b^2-n^2p^2\right)^3}\left(\left(1+(np-b)y+\left(\frac{\left(b^2-n^2p^2\right)^2}{8n^2p^2}\right)y^2\right)e^{-npy}-e^{-by}\right)\sin(npx) \quad (20)$$

Then the final solution for w_0 is,

$$w_0 = \sum_{n=1}^{\infty}\frac{2(-1)^n npb}{\left(b^2-n^2p^2\right)^2}\left(\left(\frac{8n^3p^3(b-np)+\left(b^2-n^2p^2\right)^2}{4n^2p^2\left(b^2-n^2p^2\right)}-\frac{\left(b^2-n^2p^2\right)}{2np}y\right)e^{-npy}-e^{-by}\right)\sin(npx) \quad (21)$$

Solution for w_1

The second order terms have the relation given in equation (6),

$$\nabla^2 w_1 = y_{0y} w_{0x} - y_{0x} w_{0y}$$

Substituting the solutions for y_0 and w_0 into (6),

$$\nabla^2 w_1 = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left\{F_n' G_m mp \sin(npx)\cos(mpx) - F_n G_m' np \sin(mpx)\cos(npx)\right\} \tag{22}$$

Where,

$$F_n = \frac{-2(-1)^n np\, b}{\left(b^2 - n^2 p^2\right)^3}\left(\left(1 + (np - b)y + \left(\frac{\left(b^2 - n^2 p^2\right)^2}{8n^2 p^2}\right)y^2\right)e^{-npy} - e^{-by}\right)$$

$$G_m = \left(C_{m1} e^{-mpy} - \frac{g_1}{2mp} y e^{-mpy} - \frac{g_1}{b^2 - m^2 p^2} e^{-by}\right)$$

By switching the order of summation of the second term, and by substituting $w_1 = \sum_{l=1}^{\infty}(H_l)\sin(lpx)$, the relation can be written as,

$$\sum_{l=1}^{\infty}\left(H_l'' - l^2 p^2 H_l\right)\sin(lpx) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left\{\left[F_n' G_m - F_m G_n'\right] mp \sin(npx)\cos(mpx)\right\} \tag{23}$$

$$= \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left\{\left[F_n' G_m - F_m G_n'\right]\frac{mp}{2}\left(\sin(n+m) + \sin(n-m)\right)\right\}$$

Multiply by $\sin(lpx)$ and integrate to get the relation,

$$H_l'' - l^2 p^2 H_l = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\left\{\left[F_n' G_m - F_m G_n'\right]\frac{mp}{2}\left(d_{n+m,l} + d_{n-m,l}\right)\right\}$$

$$= \sum_{m=1}^{l-1}\frac{mp}{2}\left(F_{l-m}' G_m - F_m G_{l-m}'\right) + \sum_{m=1}^{\infty}\frac{mp}{2}\left(F_{l+m}' G_m - F_m G_{l+m}'\right) \tag{24}$$

$$H_l'' - l^2 p^2 H_l = \sum_{m=1}^{l-1} \left\{ \begin{array}{l} \left(\Gamma_1 y^2 + \Gamma_2 y + \Gamma_3\right) e^{-(b+mp)y} + \left(\Gamma_4 y^3 + \Gamma_5 y^2 + \Gamma_6 y + \Gamma_7\right) e^{-lpy} + \\ \left(\Gamma_8\right) e^{-2by} + \left(\Gamma_9 y^2 + \Gamma_{10} y + \Gamma_{11}\right) e^{-(b+(l-m)p)y} \end{array} \right\}_{n=l-m} \quad (25)$$

$$+ \sum_{m=1}^{\infty} \left\{ \begin{array}{l} \left(\Gamma_1 y^2 + \Gamma_2 y + \Gamma_3\right) e^{-(b+mp)y} + \left(\Gamma_4 y^3 + \Gamma_5 y^2 + \Gamma_6 y + \Gamma_7\right) e^{-(l+2m)py} + \\ \left(\Gamma_8\right) e^{-2by} + \left(\Gamma_9 y^2 + \Gamma_{10} y + \Gamma_{11}\right) e^{-(b+(l+m)p)y} \end{array} \right\}_{n=l+m}$$

Because equation (25) is linear, a particular solution can be found for each of the terms in the summation leading to the solution given in (26). The definitions of the Φ coefficients where determined using Maple, and the Maple program output has been attached as an appendix. The solution generation procedure involved solving for each particular solution individually utilizing the Maple ODE solver. The particular solutions had to be found individually because of prohibitively long computation times required to solve the entire ODE at once. This is allowed since the problem is linear. The solution of 25 is then given by ,

$$H_l = z_1 e^{-lpy} + \sum_{m=1}^{l-1} \left\{ \begin{array}{l} \left(\Phi_1 y^2 + \Phi_2 y + \Phi_3\right) e^{-(b+mp)y} + \left(\Phi_4 y^4 + \Phi_5 y^3 + \Phi_6 y^2 + \Phi_7 y\right) e^{-lpy} + \\ \left(\Phi_8\right) e^{-2by} + \left(\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}\right) e^{-(b+(l-m)p)y} \end{array} \right\}_{n=l-m}$$

$$+ \sum_{m=1}^{\infty} \left\{ \begin{array}{l} \left(\Phi_1 y^2 + \Phi_2 y + \Phi_3\right) e^{-(b+mp)y} + \left(\Phi_4 y^3 + \Phi_5 y^2 + \Phi_6 y + \Phi_7\right) e^{-(l+2m)py} + \\ \left(\Phi_8\right) e^{-2by} + \left(\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}\right) e^{-(b+(l+m)p)y} \end{array} \right\}_{n=l+m}$$

The solution for w_1 then becomes,

$$w_1 = \sum_{n=1}^{\infty} \left(\begin{array}{l} z_1 e^{-lpy} + \sum_{m=1}^{l-1} \left\{ \begin{array}{l} \left(\Phi_1 y^2 + \Phi_2 y + \Phi_3\right) e^{-(b+mp)y} + \left(\Phi_4 y^4 + \Phi_5 y^3 + \Phi_6 y^2 + \Phi_7 y\right) e^{-lpy} + \\ \left(\Phi_8\right) e^{-2by} + \left(\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}\right) e^{-(b+(l-m)p)y} \end{array} \right\}_{n=l-m} \\ + \sum_{m=1}^{\infty} \left\{ \begin{array}{l} \left(\Phi_1 y^2 + \Phi_2 y + \Phi_3\right) e^{-(b+mp)y} + \left(\Phi_4 y^3 + \Phi_5 y^2 + \Phi_6 y + \Phi_7\right) e^{-(l+2m)py} + \\ \left(\Phi_8\right) e^{-2by} + \left(\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}\right) e^{-(b+(l+m)p)y} \end{array} \right\}_{n=l+m} \end{array} \right) \sin(npx) \quad (26)$$

Where the definitions of the Γ, Φ, and h coefficients can be found in appendix C, as determined by the Maple ODE solver.

Solution for y_1

The relation between the stream function, y_1, and w_1 is given by (7),

$$\nabla^2 y_1 = -w_1$$

Let y_1 be represented by the infinite series,

$$y_1 = \sum_{l=1}^{\infty} (K_l) \sin(lpx)$$

Substituting the solution for w_1 and the form of y_1 into (7),

$$K_l'' - l^2 p^2 K_l = -z_1 e^{-lpy} - \sum_{m=1}^{l-1} \left\{ \begin{array}{l} (\Phi_1 y^2 + \Phi_2 y + \Phi_3) e^{-(b+mp)y} + (\Phi_4 y^4 + \Phi_5 y^3 + \Phi_6 y^2 + \Phi_7 y) e^{-lpy} + \\ (\Phi_8) e^{-2by} + (\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}) e^{-(b+(l-m)p)y} \end{array} \right\}_{n=l-m}$$

$$- \sum_{m=1}^{\infty} \left\{ \begin{array}{l} (\Phi_1 y^2 + \Phi_2 y + \Phi_3) e^{-(b+mp)y} + (\Phi_4 y^3 + \Phi_5 y^2 + \Phi_6 y + \Phi_7) e^{-(l+2m)py} + \\ (\Phi_8) e^{-2by} + (\Phi_9 y^2 + \Phi_{10} y + \Phi_{11}) e^{-(b+(l+m)p)y} \end{array} \right\}_{n=l+m}$$

Again, the solution for K_l was found using the Maple ODE solver and the Maple output has been included as an appendix. The solution for K_l was found to be,

$$K_l = (z_2 + z_3 y) e^{-lpy} + \sum_{m=1}^{l-1} \left\{ \begin{array}{l} (h_1 y^2 + h_2 y + h_3) e^{-(b+mp)y} + (h_4 y^5 + h_5 y^4 + h_6 y^3 + h_7 y^2 + h_8 y) e^{-lpy} + \\ (h_9) e^{-2by} + (h_{10} y^2 + h_{11} y + h_{12}) e^{-(b+(l-m)p)y} \end{array} \right\}_{n=l-m} \quad (27)$$

$$+ \sum_{m=1}^{\infty} \left\{ \begin{array}{l} (h_1 y^2 + h_2 y + h_3) e^{-(b+mp)y} + (h_4 y^3 + h_5 y^2 + h_6 y + h_7) e^{-(l+2m)py} + \\ (h_8) e^{-2by} + (h_9 y^2 + h_{10} y + h_{11}) e^{-(b+(l+m)p)y} \end{array} \right\}_{n=l+m}$$

Applying the boundary condition $y\big|_{y=0} = 0$, (bc3), equation (27) becomes,

$$0 = z_2 + \sum_{m=1}^{l-1} \{h_3 + h_9 + h_{12}\}_{n=l-m} + \sum_{m=1}^{\infty} \{h_3 + h_7 + h_8 + h_{11}\}_{n=l+m}$$

Applying the boundary condition $y_y\big|_{y=0} = 0$, (bc3), equation (27) becomes,

$$\begin{aligned} 0 = z_3 - lp z_2 &+ \sum_{m=1}^{l-1} \{(h_2 + h_8 + h_{11}) - ((mp + b)h_3 + (2b)h_9 + (b + lp - mp)h_{12})\}_{n=l-m} \\ &+ \sum_{m=1}^{\infty} \{(h_2 + h_6 + h_{10}) - ((mp + b)h_3 + (l + 2m)p\, h_7 + (2b)h_8 + (b + lp + mp)h_{11})\}_{n=l+m} \end{aligned}$$

The required values for z_2 and z_3 are then,

$$z_2 = -\sum_{m=1}^{l-1} \{h_3 + h_9 + h_{12}\}_{n=l-m} - \sum_{m=1}^{\infty} \{h_3 + h_7 + h_8 + h_{11}\}_{n=l+m}$$

$$\begin{aligned} z_3 = &\sum_{m=1}^{l-1} \{((mp + b - lp)h_3 + (2b - lp)h_9 + (b - mp)h_{12}) - (h_2 + h_8 + h_{11})\}_{n=l-m} \\ &+ \sum_{m=1}^{\infty} \{((mp + b - lp)h_3 + (2mp)h_7 + (2b - lp)h_8 + (b + mp)h_{11}) - (h_2 + h_6 + h_{10})\}_{n=l+m} \end{aligned}$$

The exact Solution for y_1 is then,

$$y_1 = \sum_{l=1}^{\infty} \left\{ \begin{array}{l} \displaystyle\sum_{m=1}^{l-1} \left\{ \begin{array}{l} (h_1 y^2 + h_2 y + h_3)e^{-(b+mp)y} + (h_4 y^5 + h_5 y^4 + h_6 y^3 + h_7 y^2 + h_8 y)e^{-lpy} \\ + (h_9)e^{-2by} + (h_{10} y^2 + h_{11} y + h_{12})e^{-(b+(l-m)p)y} - (h_3 + h_9 + h_{12})e^{-lpy} \\ + ((mp + b - lp)h_3 + (2b - lp)h_9 + (b - mp)h_{12} - (h_2 + h_8 + h_{11}))ye^{-lpy} \end{array} \right\}_{n=l-m} \\ + \displaystyle\sum_{m=1}^{\infty} \left\{ \begin{array}{l} (h_1 y^2 + h_2 y + h_3)e^{-(b+mp)y} + (h_4 y^3 + h_5 y^2 + h_6 y + h_7)e^{-(l+2m)py} + \\ + (h_8)e^{-2by} + (h_9 y^2 + h_{10} y + h_{11})e^{-(b+(l+m)p)y} - (h_3 + h_7 + h_8 + h_{11})e^{-lpy} \\ + ((mp + b - lp)h_3 + (2mp)h_7 + (2b - lp)h_8 + (b + mp)h_{11} - (h_2 + h_6 + h_{10}))ye^{-lpy} \end{array} \right\}_{n=l+m} \end{array} \right\} \sin(lpx)$$

Results

The solutions of both Ψ_0 and w_0 were calculated using a Matlab code (appendix A) to compute and sum the first 50 Fourier series terms. Both solutions were plotted together for $b = \{\frac{1}{100}, \frac{1}{10}, 1, 10, 100\}$, in figures 1 through 5, and as can be seen, Ψ_0 and w_0 are quite similar for small b values but become considerably less so as b becomes large.

As b becomes large, the boundary condition (bc1) governing heat flux dictates that the region of heat transfer becomes small in proportion to the width X. For this reason the region of maximum vorticity migrates towards the corner of the crystal interface and the outer wall as b is increased. Notice that the vertical extent of the solution domain is reduced in the plots for large b, as the vertical extent of the flow structures is also reduced at these b values.

Also, readily apparent, is a region of zero vorticity located parallel to, and at approximately a constant distance from, the crystal interface, a result of the no slip boundary condition (bc 3) imposed there. It is interesting to note that the vertical location of this region appears to be b invariant, at about $Y = \frac{1}{5}$ for all examined values of b.

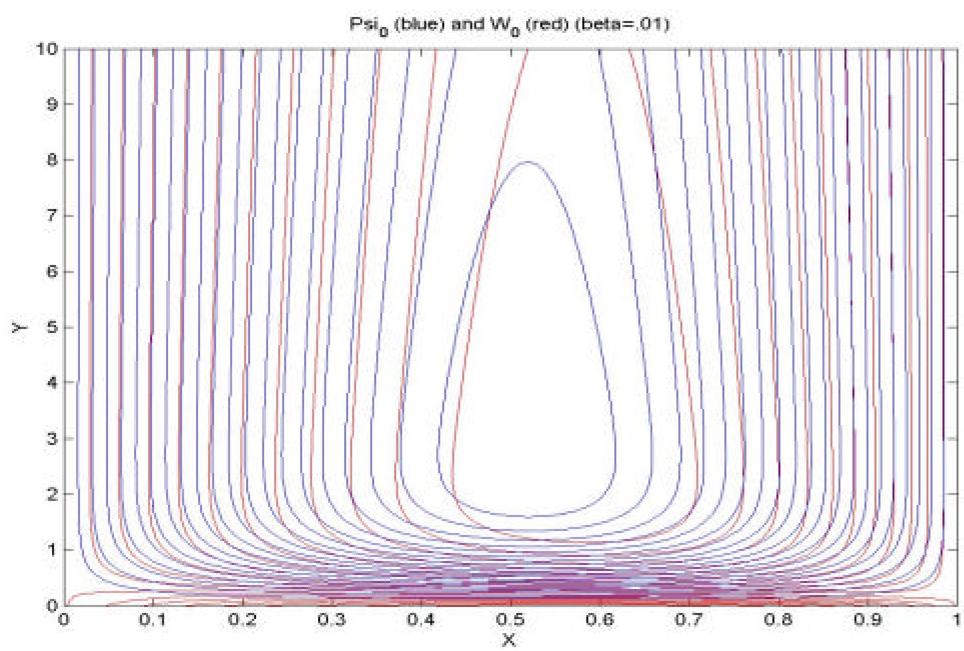

Fig 1
Ψ_0 and w_0 for b of $\frac{1}{100}$

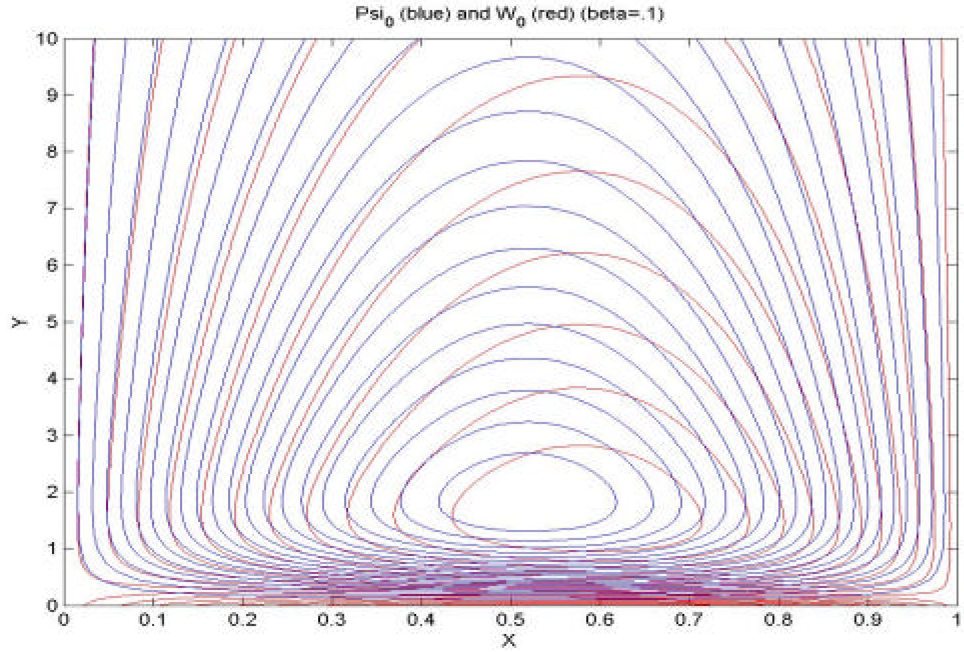

Fig 2
Ψ_0 and w_0 for b of $\frac{1}{10}$

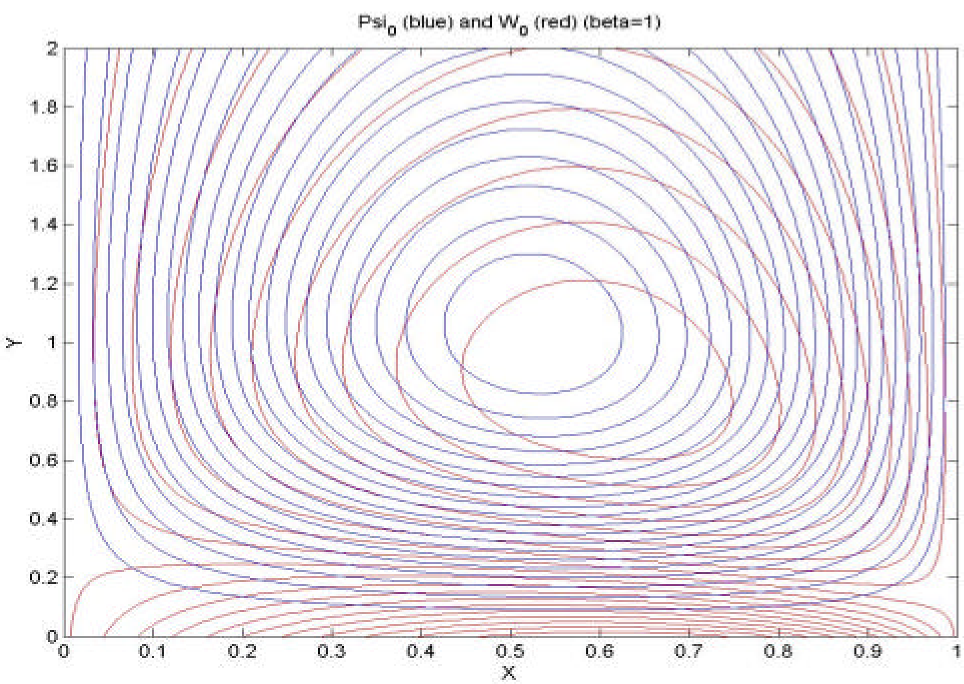

Fig 3
Ψ_0 and w_0 for b of 1

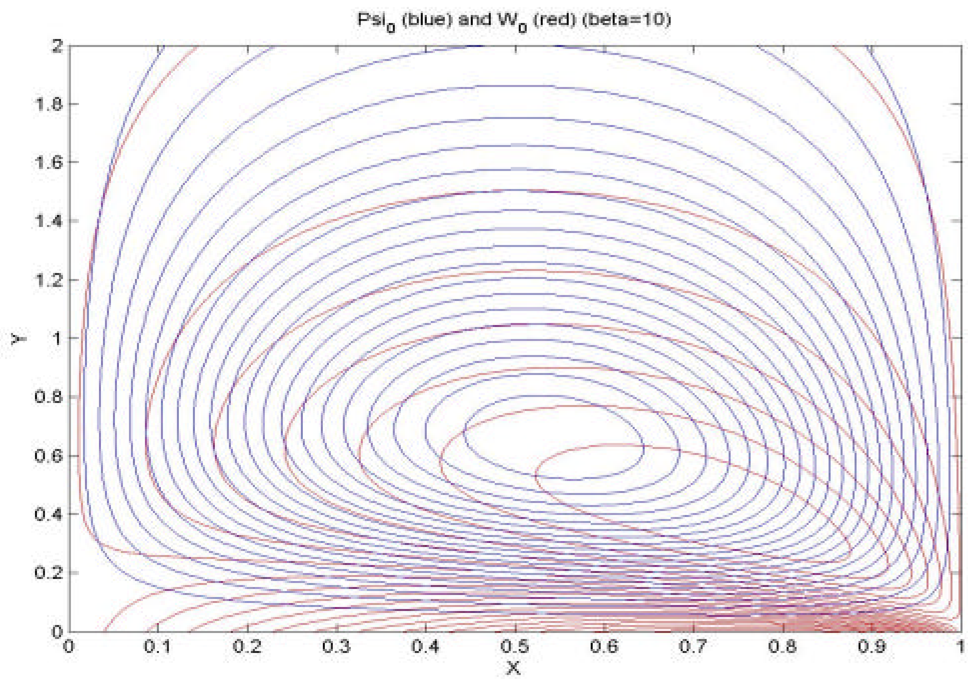

Fig 4
Ψ_0 and w_0 for b of 10

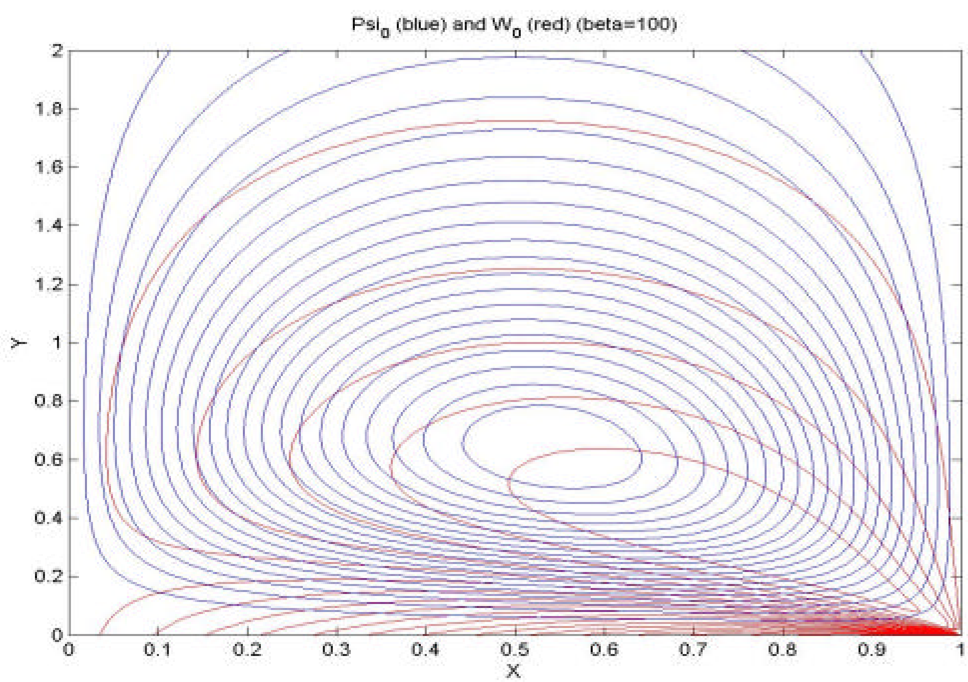

Fig 5
Ψ_0 and w_0 for b of 100

Because it is the cross terms, $\psi_{0y}\omega_{0x} - \psi_{0x}\omega_{0y}$, in equation 6 which drive the solution of Ψ_1, the value of these terms was computed to the 50th term in the Fourier series and for a set of $\beta = \{\frac{1}{100}, \frac{1}{10}, 1, 10, 100\}$. The calculation and plotting of these terms, as depicted in figures 6 through 10, was done in Matlab (appendix B). The behavior of these driving terms as a function of β, was much as expected considering the heat flux boundary condition imposed on the solution. As β is increased, the location of the maximum values of these driving terms migrates towards the corner of the crystal interface and the outer wall.

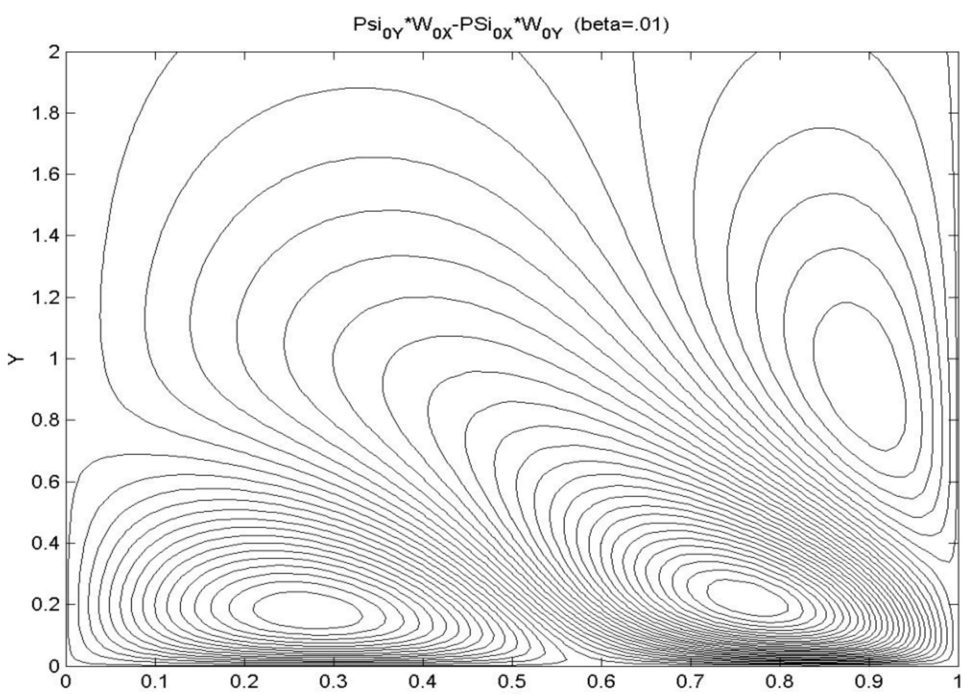

Fig 6
$\psi_{0y}\omega_{0x} - \psi_{0x}\omega_{0y}$ **for** β **of** $\frac{1}{100}$

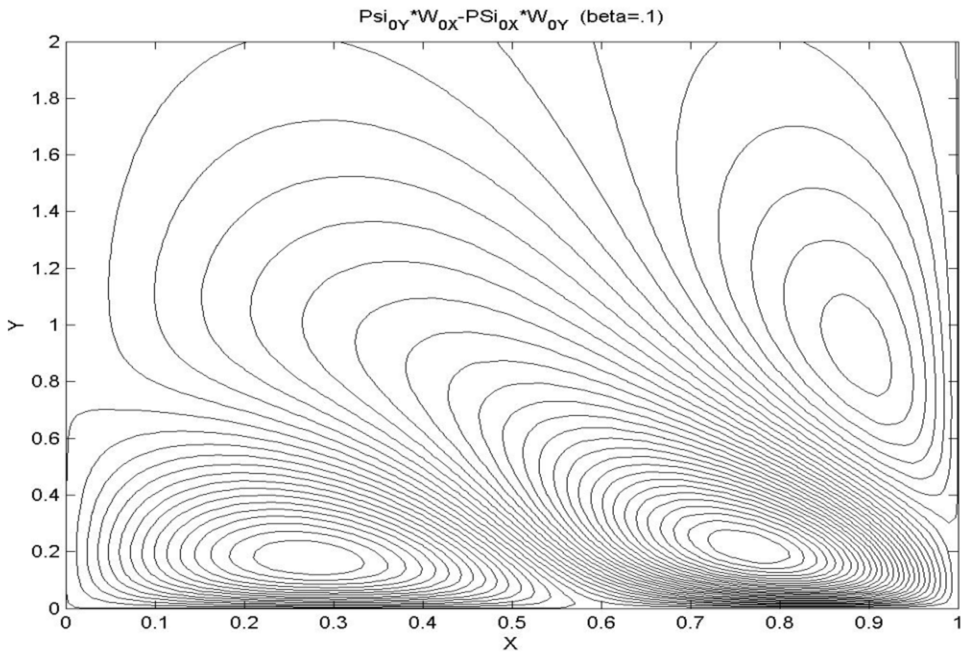

Fig 7

$y_{0y}w_{0x} - y_{0x}w_{0y}$ **for** b **of** $\frac{1}{10}$

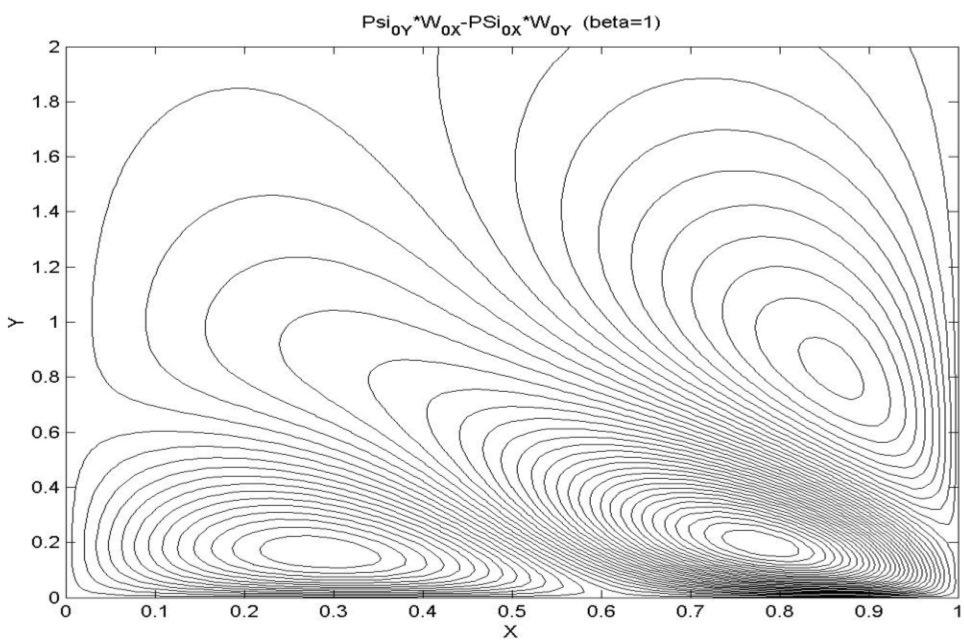

Fig 8

$y_{0y}w_{0x} - y_{0x}w_{0y}$ **for** b **of 1**

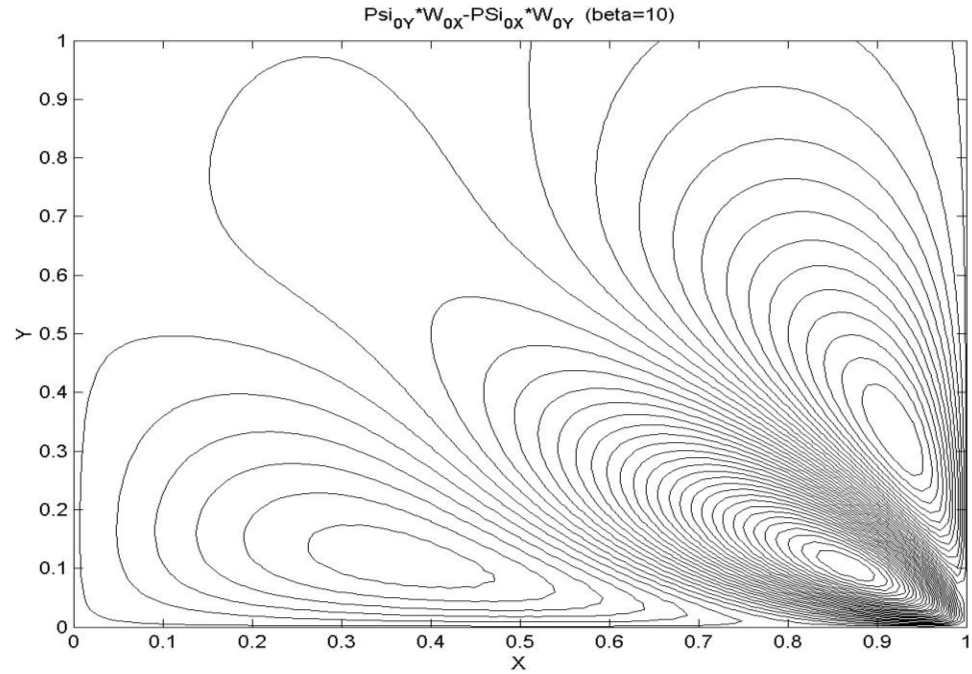

Fig 9

$\psi_{0y} w_{0x} - \psi_{0x} w_{0y}$ **for** β **of 10**

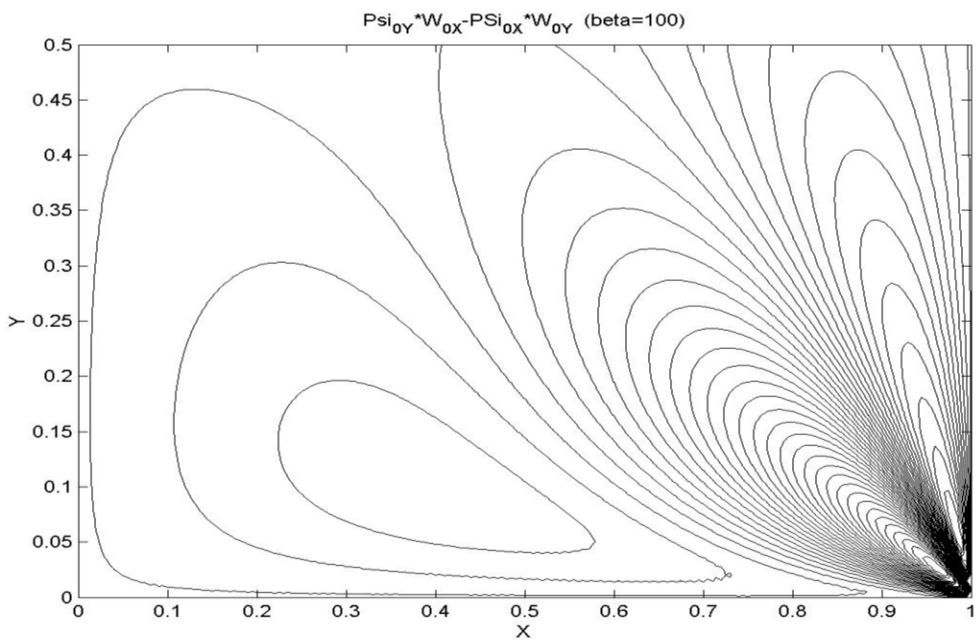

Fig 10

$\psi_{0y} w_{0x} - \psi_{0x} w_{0y}$ **for** β **of 100**

The solution for y_1 was then calculated over the same range of $b = \{\frac{1}{100}, \frac{1}{10}, 1, 10, 100\}$, and the results are given in figures 11 through 15. The calculation of y_1 was also done in Matlab (appendix C) , however, the coefficient definitions in the Matlab code were copied directly from the Maple ODE solver outputs. The solution of y_1 appears to behave well for small b , but the solution, as computed, appears to become unbounded whenever b in an integer multiple of p . This behavior is peculiar since the solution of y_1 is driven by $y_{0y}w_{0x} - y_{0x}w_{0y}$, but the solution of $y_{0y}w_{0x} - y_{0x}w_{0y}$ does not appear to be unbounded at these points, or even discontinuous.

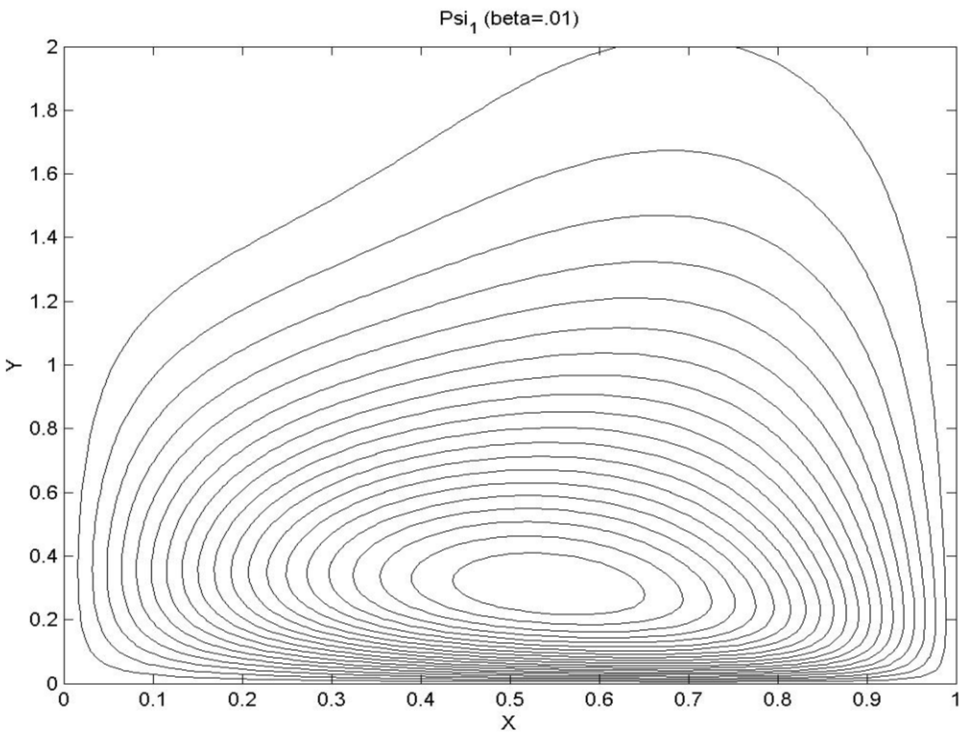

Fig 11
y_1 **for** b **of** $\frac{1}{100}$

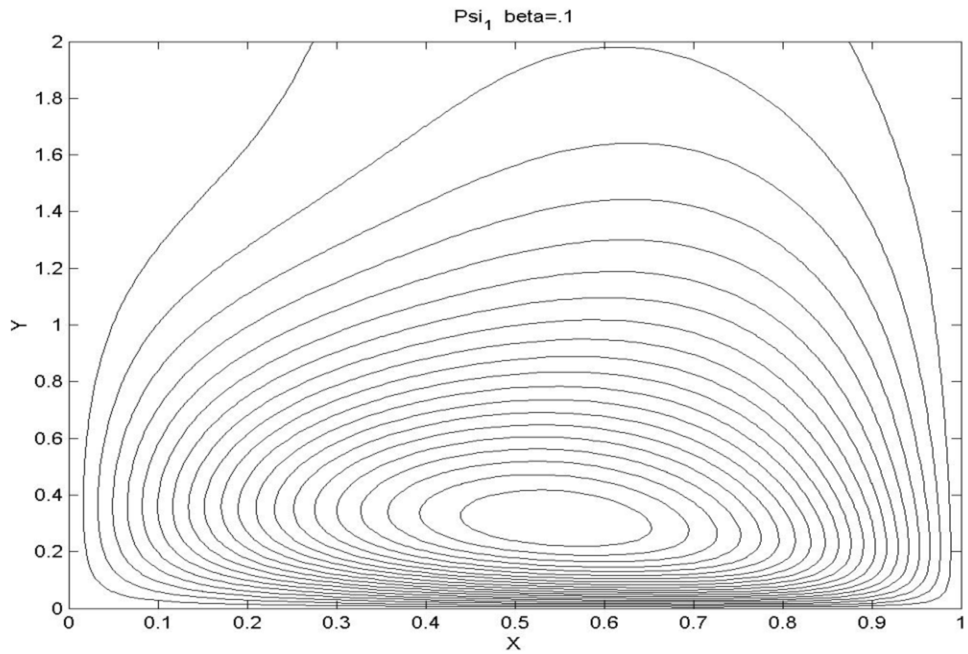

Fig 12

y_1 **for** b **of** $\frac{1}{10}$

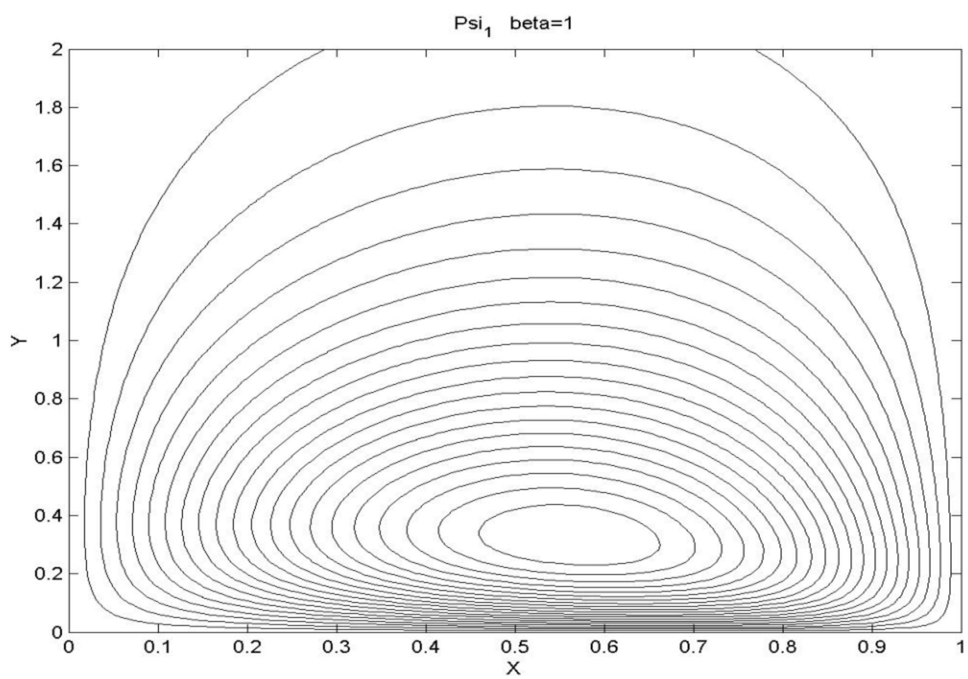

Fig 13

y_1 **for** b **of 1**

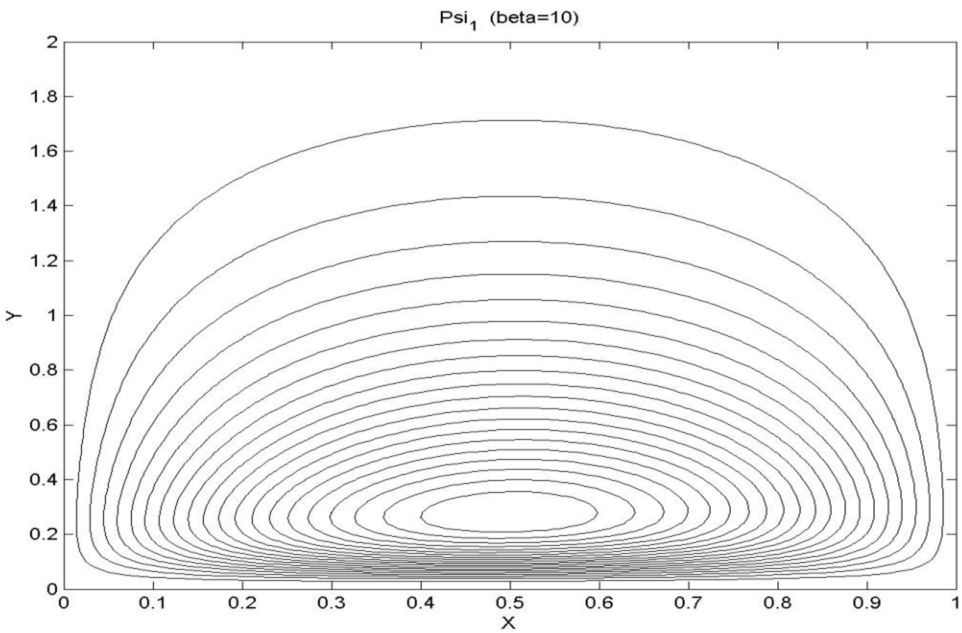

Fig 14
y_1 for b of 10

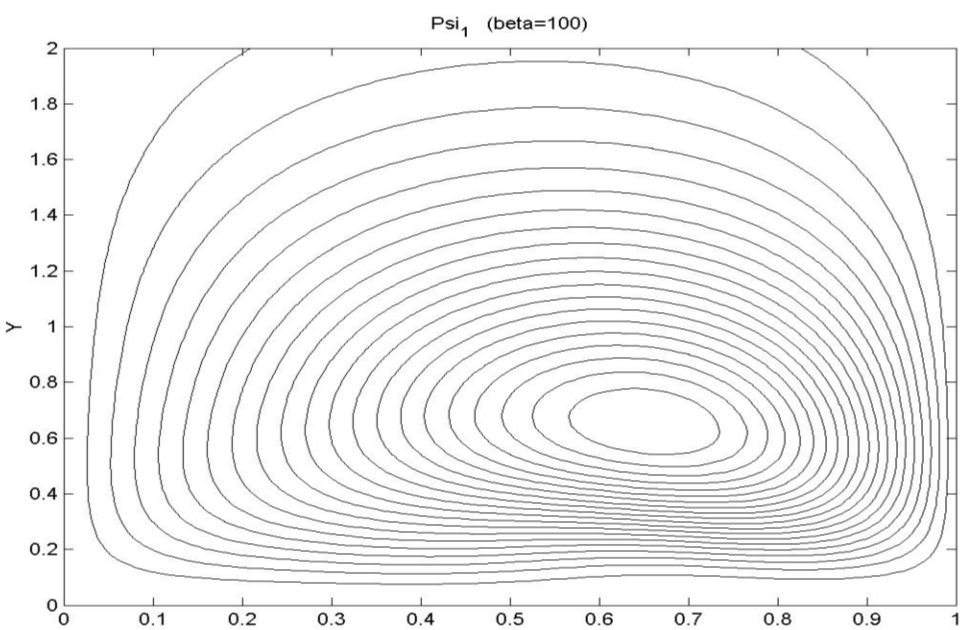

Fig 14
y_1 for b of 100

In order to better understand the relative magnitudes of the solutions of y_0, $y_{0y}w_{0x} - y_{0x}w_{0y}$, and y_1, the average absolute and maximum absolute value were recorded and plotted versus b, for b ranging from $\frac{1}{10}$ to 10. The results of this calculation are depicted in figures 16 through 18.

The singular points in the solution of y_1 can clearly be seen in figure 18, and, at present, no explanation can be offered for there existence. The process of generating the formulation of the solution using Maple and ‘cutting and pasting’ the output into Matlab for computation was carried out in such a way as to minimize any possible errors. As can be seen in appendix C, however, the resulting code is quite complex and the values of the coefficients vary widely in magnitude. It may be that the variation in magnitude of the coefficients is beyond the machine accuracy of 15 digits, and therefore information is lost during computations.

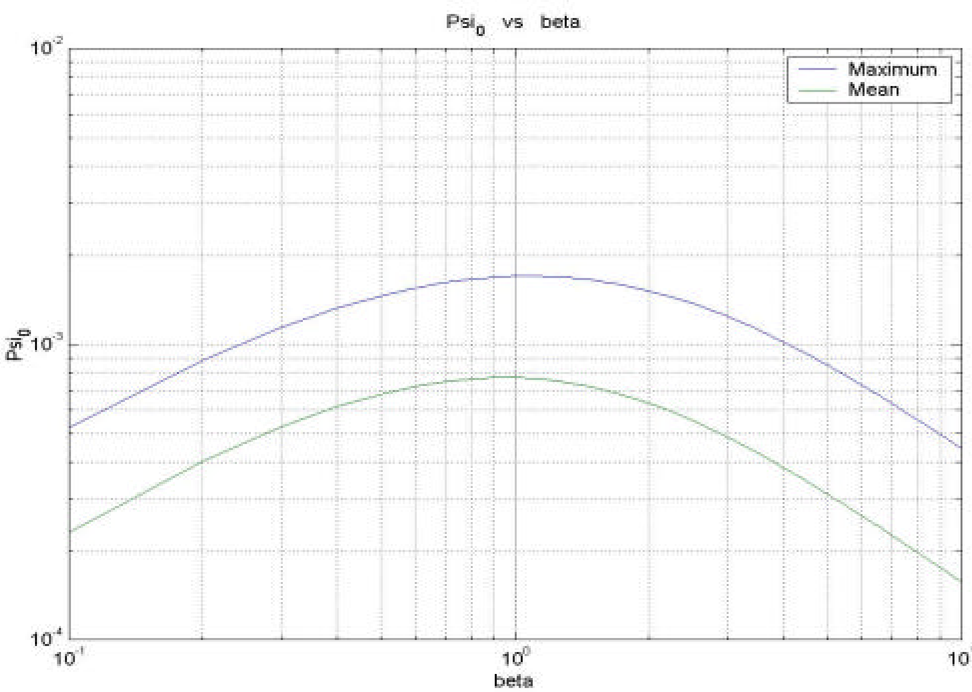

Fig 16
Maximum and Average y_0 versus b

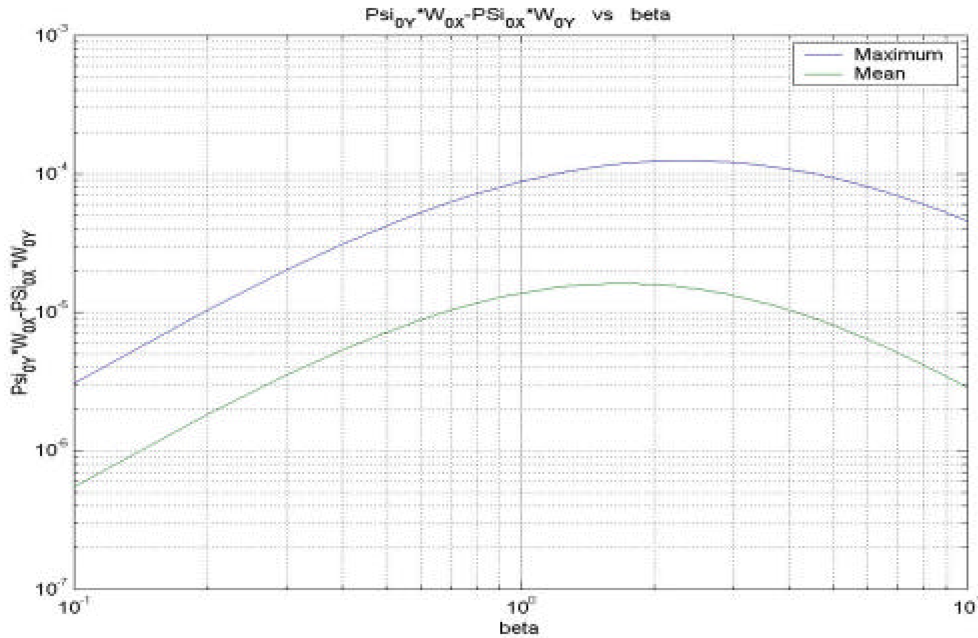

Fig 17
Maximum and Average $\psi_{0y} w_{0x} - \psi_{0x} w_{0y}$ versus β

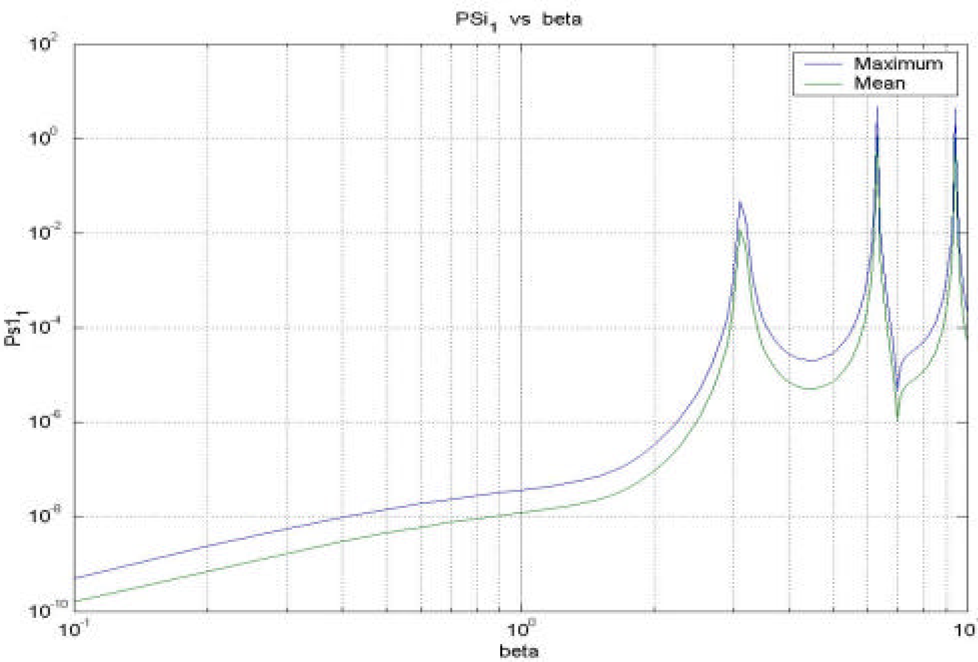

Fig 18
Maximum and Average ψ_1 versus β

This analysis finds that the order of the leading nonlinear term, y_1, is indeed substantially smaller than y_0. The ratio of y_0 to y_1, is on the order of $10^5 - 10^6$, for all values of b less than one. It is not possible to generalize the results for b greater than 1, as the solution of y_1 is unbounded at multiple points on this interval. An investigation into the genesis of these singularities in the solution of y_1 could help to better understand the true behavior of y_1 on this interval.

Qualitatively, the solution of y_0 appears to take the form of a single large eddy, nearly centered within the solution domain. Varying the value of b is essentially like varying the aspect ratio of the ampoule of melt, and thus it appears as though the solution of y_0 scales in aspect ratio with the aspect ratio of the ampoule. This is in contrast to the solution of y_1 which appears to remain constant in aspect ratio regardless of the value of b. The solution of y_1 is, however, qualitatively similar to y_0 in that the solution is characterized by a single large eddy, roughly centered in width within the solution domain. The solution of $y_{0y}w_{0x} - y_{0x}w_{0y}$ is dominated by three structures which vary greatly in form and magnitude with variation of b. The solution of $y_{0y}w_{0x} - y_{0x}w_{0y}$ does appear to scale in aspect ratio to some degree, but not to the extent of y_0, and the shifting relative locations of the solution extrema make it difficult to determine the degree of scaling.

Considering the results for b less than one, it is clear that the effect of nonlinearity in this range of problem aspect ratios is minute in comparison to the linear solution. The reason for the smallness of the non linear effects may derive from the fact that y_0 and w_0 have very similar solutions over this range of b, causing the forcing term, $y_{0y}w_{0x} - y_{0x}w_{0y}$, to be small. Also, as noted earlier, the characteristic eddy in the solution of y_1, does not scale with ampoule aspect ratio, but rather appears to be located nearly coincident with the region of zero vorticity noted in the solution of w_0. This seems to suggest that the effects of nonlinearity, in this model problem, are largely confined to this region and hence have little effect upon the overall circulation within the melt.

Appendix A

Matlab Code for production of figures 1 through 5

```
clear
beta=100;
%---Solve and plot W_0---
pi=3.1415926535898;
for x=1:1:101
   for y=1:1:201
      xc=(x-1)/100;
      yc=(y-1)/100;
      sum=0;
      for n=1:1:50
         sum=sum+2*(-1)^n*n*pi*beta/(beta^2-n^2*pi^2)^2*(((2*n*pi*(beta-
         n*pi)+1/4*(beta^2-n^2*pi^2)^2/n^2/pi^2)/(beta^2-n^2*pi^2)-(beta^2-
         n^2*pi^2)*yc/(2*n*pi))*exp(-n*pi*yc)-exp(-beta*yc))*sin(n*pi*xc);
      end
      theta(y,x)=sum;
    end
end
xb=0:.01:1;
yb=0:.01:2;
[Xa,Ya]=meshgrid(xb,yb);
contour(Xa,Ya,theta,20,'r')
hold
%---Solve and plot Psi_0---
for x=1:1:101
   for y=1:1:201
      xc=(x-1)/100;
      yc=(y-1)/100;
      sum=0;
      for n=1:1:50
         sum=sum-2*(-1)^n*n*pi*beta/(beta^2-n^2*pi^2)^3*((1+(n*pi-beta)*yc+((beta^2-
         n^2*pi^2)^2/(8*n^2*pi^2))*yc^2)*exp(-n*pi*yc)-exp(-beta*yc))*sin(n*pi*xc);
      end
      theta(y,x)=sum;
    end
end
xb=0:.01:1;
yb=0:.01:2;
[Xa,Ya]=meshgrid(xb,yb);
contour(Xa,Ya,theta,20,'b')
max(max(abs(theta)))
title('Psi_0 (blue) and W_0 (red) (beta=100)')
xlabel('X')
ylabel('Y')
```

Appendix B

Matlab Code for production of figures 6 through 10

```
clear
beta=100;
pi=3.1415926535898;
for x=1:1:201
   for y=1:1:101
     xc=(x-1)/200;
     yc=(y-1)/200;
     %---Determine Psi_y at each point
     sumpsiy=0;
     for n=1:1:200
        sumpsiy=sumpsiy-2*(-1)^n*n*pi*beta/(beta^2-n^2*pi^2)^3*((-beta+(n*pi*(beta-n*pi)+(beta^2-n^2*pi^2)^2/(4*n^2*pi^2))*yc-
       (beta^2-n^2*pi^2)^2/(8*n*pi)*yc^2)*exp(-n*pi*yc)+beta*exp(-beta*yc))*sin(n*pi*xc);
     end
      %---Determine Psi_x at each point
     sumpsix=0;
     for n=1:1:200
        sumpsix=sumpsix-2*(-1)^n*n^2*pi^2*beta/(beta^2-n^2*pi^2)^3*((1+(n*pi-beta)*yc+((beta^2 -
       n^2*pi^2)^2/(8*n^2*pi^2))*yc^2)*exp(-n*pi*yc)-exp(-beta*yc))*cos(n*pi*xc);
     end
      %---Determine W_x at each point
     sumwx=0;
     for n=1:1:200
       sumwx=sumwx+2*(-1)^n*n^2*pi^2*beta/(beta^2-n^2*pi^2)*(((2*n*pi*(beta-n*pi))/(beta^2-n^2*pi^2)^2+1/(4*n^2*pi^2)-
       yc/(2*n*pi))*exp(-n*pi*yc)-1/(beta^2-n^2*pi^2)*exp(-beta*yc))*cos(n*pi*xc);
     end
      %---Determine W_y at each point
     sumwy=0;
     for n=1:1:200
        sumwy=sumwy+2*(-1)^n*n*pi*beta/(beta^2-n^2*pi^2)*((2*n^2*pi^2*(n*pi-beta)/(beta^2-n^2*pi^2)^2-3/(4*n*pi)+yc/2)*exp(-
       n*pi*yc)+beta/(beta^2-n^2*pi^2)*exp(-beta*yc))*sin(n*pi*xc);
    end
    theta(y,x)=sumpsiy*sumwx-sumpsix*sumwy;
   end
end
xb=0:.005:1;
yb=0:.005:.5;
[Xa,Ya]=meshgrid(xb,yb);
contour(Xa,Ya,theta,40,'k')
max(max(abs(theta)))
title('Psi_0_Y*W_0_X-PSi_0_X*W_0_Y  (beta=100)')
xlabel('X')
ylabel('Y')
```

Appendix C

Matlab Code for production of figures 11 through 15

```
clear
pi=3.1415926535898;
beta=10;
for x=1:1:101
   for y=1:1:201
      xc=(x-1)/100;
      yc=(y-1)/100;
      sum=0;
      for l=1:1:10
         %---Determine n=l-m summation---
         sum1=0;
         for m=1:1:l-1
            n=l-m;
            % --Lambdas--
            Xm1 = -2*beta*m*pi*(-1)^m/(beta^2-m^2*pi^2)^3;
            Xn1 = -2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^3;
            Xm2 = 2*beta*m*pi*(beta-m*pi)*(-1)^m/(beta^2 -m^2*pi^2)^3;
            Xn2 = 2*beta*n*pi*(beta-n*pi)*(-1)^n/(beta^2 -n^2*pi^2)^3;
            Xm3 = -(-1)^m*beta/4/m/pi/(beta^2-m^2*pi^2);
            Xn3 = -(-1)^n*beta/4/n/pi/(beta^2-n^2*pi^2);
            Xm4 = 2*beta*m*pi*(-1)^m/(beta^2 -m^2*pi^2)^3;
            Xn4 = 2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^3;
            Xm5 = 2*beta*(-1)^m/(beta^2 -m^2*pi^2)^3/m /pi*(2*m^3*pi^3*(beta-m*pi)+(beta^2 -m^2*pi^2)^2/4);
            Xn5 = 2*beta*(-1)^n/(beta^2 -n^2*pi^2)^3/n/pi*(2*n^3*pi^3*(beta-n*pi)+(beta^2-n^2*pi^2)^2/4);
            Xm6 = -beta*(-1)^m/(beta^2 -m^2*pi^2);
            Xn6 = -beta*(-1)^n/(beta^2-n^2*pi^2);
            Xm7 = -2*beta*m*pi*(-1)^m/(beta^2-m^2*pi^2)^2;
            Xn7 = -2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^2;
            % --Gammas--
            Gamma1 = 1/2*m*pi*beta*Xn7*Xm3;
            Gamma2 = 1/2*m*pi*beta*(Xn7*Xm2-Xn4*Xm6);
            Gamma3 = 1/2*m*pi*beta*(Xn7*Xm1-Xn4*Xm5);
            Gamma4 = 1/2*m*n*pi^2*(Xn6*Xm3-Xn3*Xm6);
            Gamma5 = 1/2*m*pi*(Xm2*Xn6*n*pi+Xm3*Xn5*n*pi-Xm6*Xn2*n*pi-Xm3*Xn6+2*Xm6*Xn3-Xn3*n*pi*Xm5);
            Gamma6 = 1/2*m*pi*(Xm1*Xn6*n*pi+Xm2*Xn5*n*pi-Xm6*Xn1*n*pi-Xm2*Xn6+2*Xm5*Xn3-
               Xm5*Xn2*n*pi+Xm6*Xn2);
            Gamma7 = 1/2*m*pi*(-Xm5*Xn1*n*pi+Xm1*Xn5*n*pi+Xm5*Xn2-Xm1*Xn6);
            Gamma8 = 1/2*m*pi*beta*(Xm4*Xn7-Xn4*Xm7);
            Gamma9 = -1/2*m*n*pi^2*Xm7*Xn3;
            Gamma10 = 1/2*m*pi*(2*Xm7*Xn3+Xm4*Xn6*n*pi-Xm7*Xn2*n*pi);
            Gamma11 = 1/2*m*pi*(Xm7*Xn2-Xm4*Xn6+Xm4*Xn5*n*pi-Xm7*Xn1*n*pi);
            % --Phis--
            Phi1 =((l-m)^2*(l+m)^2*pi^4-4*m*(l-m)*(l+m)*beta*pi^3+4*beta^3*m*pi+(6*m^2 -
               2*l^2)*beta^2*pi^2+beta^4)*Gamma1/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
            Phi2 = ((-4*(l^2-3*m^2)*beta*pi^2 -4*m*(l-
               m)*(l+m)*pi^3+12*beta^2*m*pi+4*beta^3)*Gamma1+((l+m)*pi+beta)*(2*beta*m*pi+beta^2+(m^2-
               l^2)*pi^2)*Gamma2*((m-l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
            Phi3 =
               ((6*beta^2+12*beta*m*pi+(2*l^2+6*m^2)*pi^2)*Gamma1+((l+m)*pi+beta)*((2*beta+2*m*pi)*Gamma2+((l+m)*pi+
               beta)*Gamma3*((m-l)*pi+beta))*((m-l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
            Phi4 = -1/8*1/l/pi*Gamma4;
            Phi5 = -1/8*(2*l^2*pi^2*Gamma4+4/3*pi^3*l^3*Gamma5)/pi^4/l^4;
            Phi6 = -1/8*(3*pi*l*Gamma4+2*pi^3*l^3*Gamma6+2*l^2*pi^2*Gamma5)/pi^4/l^4;
            Phi7 = -1/8*(3*Gamma4+4*pi^3*l^3*Gamma7+2*pi^2*l^2*Gamma6+2*pi*l*Gamma5)/pi^4/l^4;
            Phi8 = 1/(-l^2*pi^2+4*beta^2)*Gamma8;
            Phi9 = (4*(l-1/2*m)^2*m^2*pi^4+4*beta^3*(l-m)*pi+4*(-3*l*m+l^2+3/2*m^2)*beta^2*pi^2-8*(l-1/2*m)*beta*(l-
               m)*m*pi^3+beta^4)*Gamma9/(beta-m*pi)^3/((2*l-m)*pi+beta)^3;
            Phi10 = ((8*(-3*l*m+l^2+3/2*m^2)*beta*pi^2-8*(l-1/2*m)*(l-m)*m*pi^3+4*beta^3+12*beta^2*(l-
               m)*pi)*Gamma9+(beta-m*pi)*(2*beta*(l-m)*pi+beta^2 -2*(l-1/2*m)*m*pi^2)*Gamma10*((2*l-m)*pi+beta))/(beta-
               m*pi)^3/((2*l-m)*pi+beta)^3;
            Phi11 = ((6*beta^2+12*beta*(l-m)*pi+( -12*l*m+8*l^2+6*m^2)*pi^2)*Gamma9+(beta-m*pi)*((2*beta+2*(l-
               m)*pi)*Gamma10+Gamma11*(beta-m*pi)*((2*l-m)*pi+beta))*((2*l-m)*pi+beta))/(beta-m*pi)^3/((2*l-m)*pi+beta)^3;
            % --Etas--
            eta1 = ((l-m)^2*(l+m)^2*pi^4-4*m*(l-m)*(l+m)*beta*pi^3+4*beta^3*m*pi+(6*m^2 -
               2*l^2)*beta^2*pi^2+beta^4)*Phi1/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
```

```
eta2 = ((-4*(l^2 -3*m^2)*beta*pi^2-4*m*(l-
    m)*(l+m)*pi^3+12*beta^2*m*pi+4*beta^3)*Phi1+((l+m)*pi+beta)*(2*beta*m*pi+beta^2+(m^2 -l^2)*pi^2)*Phi2*((m-
    l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
eta3 =
    ((6*beta^2+12*beta*m*pi+(2*l^2+6*m^2)*pi^2)*Phi1+((l+m)*pi+beta)*((2*beta+2*m*pi)*Phi2+((l+m)*pi+beta)*Phi
    3*((m-l)*pi+beta))*((m-l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
eta4 = -1/10*1/l/pi*Phi4;
eta5 = -1/10*(5/4*l^4*pi^4*Phi5+5/2*l^3*pi^3*Phi4)/l^5/pi^5;
eta6 = -1/10*(5/4*l*(2*l^2*pi^2*Phi5+4/3*l^3*pi^3*Phi6)*pi+5*l^2*pi^2*Phi4)/l^5/pi^5;
eta7 = -1/10*(5/4*l*(3*l*pi*Phi5+2*l^2*pi^2*Phi6+2*l^3*pi^3*Phi7)*pi+15/2*l*pi*Phi4)/l^5/pi^5;
eta8 = -1/10*(15/2*Phi4+5/4*l*(3*Phi5+2*Phi7*l^2*pi^2+2*l*pi*Phi6)*pi)/l^5/pi^5;
eta9 = -1/(l^2*pi^2-4*beta^2)*Phi8;
eta10 = -1/2*(m^2*(l-1/2*m)^2*pi^4+beta^3*(l-m)*pi+(3/2*m^2-3*l*m+l^2)*beta^2*pi^2-2*(l-m)*m*beta*(l-
    1/2*m)*pi^3+1/4*beta^4)*Phi9/(m*pi-beta)^3/((l-1/2*m)*pi+1/2*beta)^3;
eta11 = -1/2*((2*(3/2*m^2-3*l*m+l^2)*beta*pi^2 -2*(l-m)*m*(l-1/2*m)*pi^3+beta^3+3*beta^2*(l-m)*pi)*Phi9+(m*pi-
    beta)*((l-1/2*m)*pi+1/2*beta)*(-beta*(l-m)*pi-1/2*beta^2+m*(l-1/2*m)*pi^2)*Phi10)/(m*pi-beta)^3/((l-
    1/2*m)*pi+1/2*beta)^3;
eta12 = -1/2*((3/2*beta^2+3*beta*(l-m)*pi+(-3*l*m+3/2*m^2+2*l^2)*pi^2)*Phi9+(m*pi-beta)*((l-
    1/2*m)*pi+1/2*beta)*((-beta-(l-m)*pi)*Phi10+Phi11*(m*pi-beta)*((l-1/2*m)*pi+1/2*beta)))/(m*pi-beta)^3/((l-
    1/2*m)*pi+1/2*beta)^3;

sum1=sum1+((eta1*yc^2+eta2*yc+eta3)*exp(-
    (beta+m*pi)*yc)+(eta4*yc^5+eta5*yc^4+eta6*yc^3+eta7*yc^2+eta8*yc)*exp(-l*pi*yc)+eta9*exp(-
    2*beta*yc)+(eta10*yc^2+eta11*yc+eta12)*exp(-(beta+(l-m)*pi)*yc)-(eta2+(l*pi-(beta+m*pi))*eta3+eta8+(l*pi-
    2*beta)*eta9+eta11+(m*pi-beta)*eta12)*yc*exp(-l*pi*yc)-(eta3+eta9+eta12)*exp(-l*pi*yc));
end
%---Determine n=l+m summation---
sum2=0;
for m=1:1:10
  n=l+m;
  % --Lambdas--
  Xm1 = -2*beta*m*pi*(-1)^m/(beta^2-m^2*pi^2)^3;
  Xn1 = -2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^3;
  Xm2 = 2*beta*m*pi*(beta-m*pi)*(-1)^m/(beta^2 -m^2*pi^2)^3;
  Xn2 = 2*beta*n*pi*(beta-n*pi)*(-1)^n/(beta^2 -n^2*pi^2)^3;
  Xm3 = -(-1)^m*beta/4/m/pi/(beta^2-m^2*pi^2);
  Xn3 = -(-1)^n*beta/4/n/pi/(beta^2-n^2*pi^2);
  Xm4 = 2*beta*m*pi*(-1)^m/(beta^2 -m^2*pi^2)^3;
  Xn4 = 2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^3;
  Xm5 = 2*beta*(-1)^m/(beta^2 -m^2*pi^2)^3/m/pi*(2*m^3*pi^3*(beta-m*pi)+(beta^2 -m^2*pi^2)^2/4);
  Xn5 = 2*beta*(-1)^n/(beta^2 -n^2*pi^2)^3/n/pi*(2*n^3*pi^3*(beta-n*pi)+(beta^2-n^2*pi^2)^2/4);
  Xm6 = -beta*(-1)^m/(beta^2 -m^2*pi^2);
  Xn6 = -beta*(-1)^n/(beta^2 -n^2*pi^2);
  Xm7 = -2*beta*m*pi*(-1)^m/(beta^2-m^2*pi^2)^2;
  Xn7 = -2*beta*n*pi*(-1)^n/(beta^2 -n^2*pi^2)^2;
  % --Gammas--
  Gamma1 = 1/2*m*pi*beta*Xn7*Xm3;
  Gamma2 = 1/2*m*pi*beta*(Xn7*Xm2-Xn4*Xm6);
  Gamma3 = 1/2*m*pi*beta*(Xn7*Xm1-Xn4*Xm5);
  Gamma4 = 1/2*m*n*pi^2*(Xn6*Xm3-Xn3*Xm6);
  Gamma5 = 1/2*m*pi*(Xm2*Xn6*n*pi+Xm3*Xn5*n*pi-Xm6*Xn2*n*pi-Xm3*Xn6+2*Xm6*Xn3-Xn3*n*pi*Xm5);
  Gamma6 = 1/2*m*pi*(Xm1*Xn6*n*pi+Xm2*Xn5*n*pi-Xm6*Xn1*n*pi-Xm2*Xn6+2*Xm5*Xn3-
    Xm5*Xn2*n*pi+Xm6*Xn2);
  Gamma7 = 1/2*m*pi*(-Xm5*Xn1*n*pi+Xm1*Xn5*n*pi+Xm5*Xn2-Xm1*Xn6);
  Gamma8 = 1/2*m*pi*bet a*(Xm4*Xn7-Xn4*Xm7);
  Gamma9 = -1/2*m*n*pi^2*Xm7*Xn3;
  Gamma10 = 1/2*m*pi*(2*Xm7*Xn3+Xm4*Xn6*n*pi-Xm7*Xn2*n*pi);
  Gamma11 = 1/2*m*pi*(Xm7*Xn2-Xm4*Xn6+Xm4*Xn5*n*pi-Xm7*Xn1*n*pi);
  % --Phis--
  Phi1 =((l-m)^2*(l+m)^2*pi^4-4*m*(l-m)*(l+m)*beta*pi^3+4*beta^3*m*pi+(6*m^2 -
    2*l^2)*beta^2*pi^2+beta^4)*Gamma1/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
  Phi2 = ((-4*(l^2-3*m^2)*beta*pi^2 -4*m*(l-
    m)*(l+m)*pi^3+12*beta^2*m*pi+4*beta^3)*Gamma1+((l+m)*pi+beta)*(2*beta*m*pi+beta^2+(m^2-
    l^2)*pi^2)*Gamma2*((m-l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
  Phi3 =
    ((6*beta^2+12*beta*m*pi+(2*l^2+6*m^2)*pi^2)*Gamma1+((l+m)*pi+beta)*((2*beta+2*m*pi)*Gamma2+((l+m)*pi+
    beta)*Gamma3*((m-l)*pi+beta))*((m-l)*pi+beta))/((l+m)*pi+beta)^3/((m-l)*pi+beta)^3;
  Phi4 = 1/4*(3*l^2*pi^3*m^4+l^3*pi^3*m^3+pi^3*m^6+3*l*pi^3*m^5)*Gamma4/pi^5/m^4/(l+m)^4;
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            Phi5 =
                1/4*((15/2*l*pi^2*m^4+6*l^2*pi^2*m^3+3/2*l^3*pi^2*m^2+3*pi^2*m^5)*Gamma4+(l+m)*pi*(l^2*pi^2*m^2+2*l*
                pi^2*m^3+m^4*pi^2)*Gamma5*m)/pi^5/m^4/(l+m)^4;
            Phi6 =
                1/4*((3/2*l^3*pi*m+9/2*pi*m^4+9*l*pi*m^3+6*l^2*pi*m^2)*Gamma4+(l+m)*pi*((2*pi*m^3+3*l*pi*m^2+l^2*pi*
                m)*Gamma5+(l+m)*pi*(pi*l*m+m^2*pi)*Gamma6*m)*m)/pi^5/m^4/(l+m)^4;
            Phi7 =
                1/4*((3*l^2*m+3/4*l^3+3*m^3+9/2*l*m^2)*Gamma4+(l+m)*pi*((1/2*l^2+3/2*l*m+3/2*m^2)*Gamma5+(l+m)*pi*((
                1/2*l+m)*Gamma6+pi*m*Gamma7*(l+m))*m)*m)/pi^5/m^4/(l+m)^4;
            Phi8 = 1/(-l^2*pi^2+4*beta^2)*Gamma8;
            Phi9 =
                (4*(l+1/2*m)^2*m^2*pi^4+4*beta^3*(l+m)*pi+4*(3/2*m^2+3*l*m+l^2)*beta^2*pi^2+8*(l+m)*(l+1/2*m)*beta*m*pi
                ^3+beta^4)*Gamma9/((2*l+m)*pi+beta)^3/(beta+m*pi)^3;
            Phi10 =
                ((8*(3/2*m^2+3*l*m+l^2)*beta*pi^2+8*(l+m)*(l+1/2*m)*m*pi^3+4*beta^3+12*beta^2*(l+m)*pi)*Gamma9+(2*beta
                *(l+m)*pi+beta^2+2*(l+1/2*m)*m*pi^2)*Gamma10*((2*l+m)*pi+beta)*(beta+m*pi))/((2*l+m)*pi+beta)^3/(beta+m*
                pi)^3;
            Phi11 =
                ((6*beta^2+12*beta*(l+m)*pi+(6*m^2+8*l^2+12*l*m)*pi^2)*Gamma9+((2*beta+2*(l+m)*pi)*Gamma10+((2*l+m)*
                pi+beta)*Gamma11*(beta+m*pi))*((2*l+m)*pi+beta)*(beta+m*pi))/((2*l+m)*pi+beta)^3/(beta+m*pi)^3;
            % --Etas--
            eta1 =((l-m)^2*(l+m)^2*pi^4+(-2*l^2+6*m^2)*beta^2*pi^2+4*beta^3*m*pi+beta^4-4*m*(l-
                m)*(l+m )*beta*pi^3)*Phi1/((l+m)*pi+beta)^3/((l-m)*pi+beta)^3;
            eta2 = ((-4*(l^2 -3*m^2)*beta*pi^2-4*m*(l-m)*(l+m)*pi^3+4*beta^3+12*beta^2*m*pi)*Phi1+((l+m)*pi+beta)*(-
                2*beta*m*pi-beta^2+(-m^2+l^2)*pi^2)*Phi2*((l-m)*pi-beta))/((l+m)*pi+beta)^3/((l-m)*pi+beta)^3;
            eta3 = ((12*beta*m*pi+(2*l^2+6*m^2)*pi^2+6*beta^2)*Phi1+((l+m)*pi+beta)*((-2*beta-
                2*m*pi)*Phi2+Phi3*((l+m)*pi+beta)*((l-m)*pi-beta))*((l-m)*pi-beta))/((l+m)*pi+beta)^3/((l-m)*pi+beta)^3;
            eta4 = 1/4*(3*l^2*pi^3*m^4+l^3*pi^3*m^3+pi^3*m^6+3*l*pi^3*m^5)*Phi4/pi^5/m^4/(m+l)^4;
            eta5 =
                1/4*((15/2*l*pi^2*m^4+6*l^2*pi^2*m^3+3/2*l^3*pi^2*m^2+3*pi^2*m^5)*Phi4+(m+l)*(l^2*pi^2*m^2+2*l*pi^2*m^
                3+pi^2*m^4)*Phi5*m*pi)/pi^5/m^4/(m+l)^4;
            eta6 =
                1/4*((3/2*l^3*pi*m+9/2*pi*m^4+9*l*pi*m^3+6*l^2*pi*m^2)*Phi4+(l+m)*pi*((2*pi*m^3+3*l*pi*m^2+l^2*pi*m)*P
                hi5+(l+m)*pi*(pi*l*m+m^2*pi)*Phi6*m)*m)/pi^5/m^4/(l+m)^4;
            eta7 =
                1/4*((3*l^2*m+3/4*l^3+3*m^3+9/2*l*m^2)*Phi4+(l+m)*pi*((1/2*l^2+3/2*l*m+3/2*m^2)*Phi5+(l+m)*pi*((1/2*l+m
                )*Phi6+pi*m*Phi7*(l+m))*m)*m)/pi^5/m^4/(l+m)^4;
            eta8 = 1/(-l^2*pi^2+4*beta^2)*Phi8;
            eta9 =
                (4*m^2*(l+1/2*m)^2*pi^4+8*m*(l+1/2*m)*beta*(m+l)*pi^3+4*beta^3*(m+l)*pi+4*(l^2+3*l*m+3/2*m^2)*beta^2*pi
                ^2+beta^4)*Phi9/((2*l+m)*pi+beta)^3/(beta+m*pi)^3;
            eta10 =
                ((8*(l^2+3*l*m+3/2*m^2)*beta*pi^2+8*m*(l+1/2*m)*(m+l)*pi^3+4*beta^3+12*beta^2*(m+l)*pi)*Phi9+((2*l+m)*pi
                +beta)*(beta+m*pi)*(2*beta*(m+l)*pi+beta^2+2*m*(l+1/2*m)*pi^2)*Phi10)/((2*l+m)*pi+beta)^3/(beta+m*pi)^3;
            eta11 =
                ((12*beta*(m+l)*pi+(12*l*m+6*m^2+8*l^2)*pi^2+6*beta^2)*Phi9+((2*l+m)*pi+beta)*(beta+m*pi)*((2*beta+2*(m+l
                )*pi)*Phi10+((2*l+m)*pi+beta)*Phi11*(beta+m*pi)))/((2*l+m)*pi+beta)^3/(beta+m*pi)^3;

            sum2=sum2+((eta1*yc^2+eta2*yc+eta3)*exp(-(beta+m*pi)*yc)+(eta4*yc^3+eta5*yc^2+eta6*yc+eta7)*exp(-
                (l+2*m)*pi*yc)+eta8*exp(-2*beta*yc)+(eta9*yc^2+eta10*yc+eta11)*exp(-(beta+(l+m)*pi)*yc)-(eta2+(l*pi-
                (beta+m*pi))*eta3+eta6+(-2*m*pi)*eta7+(l*pi-2*beta)*eta8+eta10+(-beta-m*pi)*eta11)*yc*exp(-l*pi*yc)-
                (eta3+eta7+eta8+eta11)*exp(-l*pi*yc));
        end
        sum=sum+(sum1+sum2)*sin(l*pi*xc);
      end
      theta(y,x)=sum;
   end
   x
end
xb=0:.01:1;
yb=0:.01:2;
[Xa,Ya]=meshgrid(xb,yb);
contour(Xa,Ya,theta,40,'k')
```

Reference

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